

Anthracene, 9-butyltetradecahydro-

Other names: 9-Butyltetradecahydroanthracene;
9-n-Butyl-(tetradecahydroanthracene).

InChI: InChI=1S/C18H32/c1-2-3-10-18-16-11-6-4-8-14(16)13-15-9-5-7-12-17(15)18/h14-18H,2-13H2,1H3

InChI Key: PJCBPQWYVHKO-UHFFFAOYSA-N

Formula: C18H32

SMILES: CCCCC1C2CCCCC2CC2CCCCC12

Molecular Weight: 248.45

CAS: 55133-89-6



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	207.01	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-267.93	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	28.42	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	55.64	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	5.81		Crippen Method
P_c	1603.85	kPa	Joback Method
T_{boil}	643.47	K	Joback Method
T_c	859.29	K	Joback Method
T_{fus}	320.36	K	Joback Method
V_c	0.87	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	702.60	J/mol×K	643.47	Joback Method
η	0.00	Paxs	643.47	Joback Method
$\Delta_{\text{vap}} H$	72.80	kJ/mol	438.0	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C18H32/c1-2-3-10-18-16-11-6-4-8-14\(16\)13-15-9-5-7-12-17\(15\)18/h14-18H,2-13H2,1H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C18H32/c1-2-3-10-18-16-11-6-4-8-14(16)13-15-9-5-7-12-17(15)18/h14-18H,2-13H2,1H3)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).

η : Dynamic viscosity (Pa×s).

$\Delta_f G^\circ$: Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{fus} H^\circ$: Enthalpy of fusion at standard conditions (kJ/mol).

$\Delta_{vap} H^\circ$: Enthalpy of vaporization at standard conditions (kJ/mol).

$\Delta_{vap} H$: Enthalpy of vaporization at a given temperature (kJ/mol).

$logP_{oct/wat}$: Octanol/Water partition coefficient .

P_c : Critical Pressure (kPa).

T_{boil} : Normal Boiling Point Temperature (K).

T_c : Critical Temperature (K).

T_{fus} : Normal melting (fusion) point (K).

V_c : Critical Volume (m³/kg-mol).

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